

# Unsupervised Analysis: Best Practices

# Exploratory vs. Confirmatory Analysis

## Confirmatory Analysis:

- Seeks to test an a priori hypothesis.
- Examples:
  - ▶ Classical inferential statistics.
  - ▶ Prediction in supervised learning.

## Exploratory Analysis:

- Seeks to make data-driven discoveries.
- Hypothesis generating.

Which is unsupervised analysis?

# Validating Data-Driven Discoveries

- Corroborate via existing literature.
- Show data-driven discovery is stable.
  - ▶ Small changes to the data, the algorithm, the method, the parameters, etc. yield the same result.
  - ▶ Multiple approaches yield the same result.
- Validate via biological experiments.
  - ▶ True confirmation.
  - ▶ Expensive & sometimes not possible.
- Confirm via a completely separate test set.

# Confirming Discoveries on a Test Set

## Exercise

Suppose you use a training data set to BLANK. How would you use a separate test data set to validate this discovery?

BLANK:

- Discover a major pattern.
- Discover clusters.
- Discover important features.
- Discover important connections between features.

# Some Good Rules for Unsupervised Analysis

- 1 Always visualize.
- 2 Use multiple techniques.
- 3 Validate discoveries when possible.
- 4 Communicate uncertainty.
- 5 Make your analysis reproducible.